*Article*

# Complex Evaluation of Antioxidant Capacity of Milk Thistle Dietary Supplements

**Jitka Viktorova [1], Milena Stranska-Zachariasova [2,*], Marie Fenclova [2], Libor Vitek [3], Jana Hajslova [2], Vladimir Kren [4] and Tomas Ruml [1]**

[1] Department of Biochemistry and Microbiology, University of Chemistry and Technology Prague, Technická 5, 166 28 Prague, Czech Republic
[2] Department of Food Analysis and Nutrition, University of Chemistry and Technology Prague, Technická 5, 166 28 Prague, Czech Republice
[3] 4th Department of Internal Medicine and Institute of Medical Biochemistry and Laboratory Diagnostics, 1st Faculty of Medicine, Charles University, Katerinska 32, 12000 Prague, Czech Republic
[4] Laboratory of Biotransformation, Institute of Microbiology, Czech Academy of Sciences, Vídeňská 1083, 142 20 Prague, Czech Republice
* Correspondence: milena.stranska@vscht.cz

**Supplementary Table** 1 List of non-silymarin bioactive compounds reported in literature for *Silybum marianum* (SM)[1, 2, 3-10], *Schisandra chinensis* (SCH)[11], *Cordyceps sinensis* (CS)[12, 13], *Scutellaria baicalensis* (SB)[14, 15], *Cnicus benedictus* (CB)[16], *Foeniculum vulgare* (FV)[17, 18], *Taraxacum officinale* (TO)[19] and *Glycyrrhiza glabra* (GG)[20].

| Compound name | Summary formula | Plant of origin |
|---|---|---|
| neusilychristin | $C_{25}H_{22}O_{10}$ | *SM* |
| silyamandin | $C_{25}H_{22}O_{11}$ | *SM* |
| isosilandrin A | $C_{25}H_{22}O_{9}$ | *SM* |
| isosilandrin B | $C_{25}H_{22}O_{9}$ | *SM* |
| neosilyhermin A | $C_{25}H_{22}O_{9}$ | *SM* |
| neosilyhermin B | $C_{25}H_{22}O_{9}$ | *SM* |
| silandrin A | $C_{25}H_{22}O_{9}$ | *SM* |
| silandrin B | $C_{25}H_{22}O_{9}$ | *SM* |
| silyhermin | $C_{25}H_{22}O_{9}$ | *SM* |
| silymonin | $C_{25}H_{22}O_{9}$ | *SM* |
| apigenin | $C_{15}H_{10}O_{5}$ | *SM* |
| genistein | $C_{15}H_{10}O_{5}$ | *SM* |
| luteolin | $C_{15}H_{10}O_{6}$ | *SM* |
| kaempferol | $C_{15}H_{10}O_{6}$ | *SM* |
| quercetin | $C_{15}H_{10}O_{7}$ | *SM* |

| | | |
|---|---|---|
| myricetin | $C_{15}H_{10}O_8$ | *SM* |
| naringenin | $C_{15}H_{12}O_5$ | *SM* |
| dihydrokaempferol (aromadendrin) | $C_{15}H_{12}O_6$ | *SM* |
| eriodictyol | $C_{15}H_{12}O_6$ | *SM* |
| catechin | $C_{15}H_{14}O_6$ | *SM* |
| acacetin | $C_{16}H_{12}O_5$ | *SM* |
| genkwanin | $C_{16}H_{12}O_5$ | *SM* |
| hispidulin | $C_{16}H_{12}O_6$ | *SM* |
| chrysoeriol | $C_{16}H_{12}O_6$ | *SM* |
| kaempferol-3-methyl ether (isokaempferide) | $C_{16}H_{12}O_6$ | *SM* |
| nepetin | $C_{16}H_{12}O_7$ | *SM* |
| rhamentin | $C_{16}H_{12}O_7$ | *SM* |
| patuletin | $C_{16}H_{12}O_8$ | *SM* |
| apigenin-5,7-dimethyl ether | $C_{17}H_{14}O_5$ | *SM* |
| pectolinarigenin | $C_{17}H_{14}O_6$ | *SM* |
| kumatakenin | $C_{17}H_{14}O_6$ | *SM* |
| jaceosidin | $C_{17}H_{14}O_7$ | *SM* |
| eupatilin | $C_{18}H_{16}O_7$ | *SM* |
| sudachitin | $C_{18}H_{16}O_8$ | *SM* |
| hymenoxin | $C_{19}H_{18}O_8$ | *SM* |
| quercetin-3-O-arabinoside | $C_{20}H_{18}O_{11}$ | *SM* |
| luteolin-7-O-glucuronide | $C_{21}H_{17}O_{12}$ | *SM* |
| apigenin-7-O-glucuronide | $C_{21}H_{18}O_{11}$ | *SM* |
| miquelianin (quercetin 3-glucoronide) | $C_{21}H_{18}O_{13}$ | *SM* |
| isovitexin | $C_{21}H_{20}O_{10}$ | *SM* |
| apigenin-7-O-glucoside | $C_{21}H_{20}O_{10}$ | *SM* |
| vitexin | $C_{21}H_{20}O_{10}$ | *SM* |
| isoorientin | $C_{21}H_{20}O_{11}$ | *SM* |
| orientin | $C_{21}H_{20}O_{11}$ | *SM* |
| kaempferol-3-O-beta-D-glucoside (astragalin) | $C_{21}H_{20}O_{11}$ | *SM* |

| | | |
|---|---|---|
| luteolin-7-O-glucoside (cynaroside) | $C_{21}H_{20}O_{11}$ | *SM* |
| quercetin 3-O-galactoside (hyperoside) | $C_{21}H_{20}O_{12}$ | *SM* |
| quercetin 3-O-glucoside (isoquercetin) | $C_{21}H_{20}O_{12}$ | *SM* |
| spiraeoside (quercetin 4-O-glucoside) | $C_{21}H_{20}O_{12}$ | *SM* |
| naringenin 7-O-beta-D-glucopyranoside | $C_{21}H_{22}O_{10}$ | *SM* |
| isokaempferide 7-rhamnoside | $C_{22}H_{22}O_{10}$ | *SM* |
| isorhamnetin 3-O-glucoside | $C_{22}H_{22}O_{12}$ | *SM* |
| apigenin-4,7-diglucoside | $C_{27}H_{30}O_{15}$ | *SM* |
| kaempferol-3-rutinoside | $C_{27}H_{30}O_{15}$ | *SM* |
| rutin | $C_{27}H_{30}O_{16}$ | *SM* |
| naringin | $C_{27}H_{32}O_{14}$ | *SM* |
| hydroxybenzoic acid (salicylic acid) | $C_{7}H_{6}O_{3}$ | *SM* |
| beta-resorcylic acid (dihydroxybenzoic acid) | $C_{7}H_{6}O_{4}$ | *SM* |
| gallic acid | $C_{7}H_{6}O_{5}$ | *SM* |
| guaiacol | $C_{7}H_{8}O_{2}$ | *SM* |
| vanillic acid | $C_{8}H_{8}O_{4}$ | *SM* |
| syringaldehyde | $C_{9}H_{10}O_{4}$ | *SM* |
| syringic acid | $C_{9}H_{10}O_{5}$ | *SM* |
| coumaric acid | $C_{9}H_{8}O_{3}$ | *SM* |
| caffeic acid | $C_{9}H_{8}O_{4}$ | *SM* |
| coniferylaldehyd | $C_{10}H_{10}O_{3}$ | *SM* |
| ferulic acid | $C_{10}H_{10}O_{4}$ | *SM* |
| dihydroconiferyl alcohol | $C_{10}H_{14}O_{3}$ | *SM* |
| ethyl caffeate | $C_{11}H_{12}O_{4}$ | *SM* |
| methyl ferulate | $C_{11}H_{12}O_{4}$ | *SM* |
| sinapinic acid | $C_{11}H_{12}O_{5}$ | *SM* |
| ellagic acid | $C_{14}H_{6}O_{8}$ | *SM* |
| 3-O-caffeoylquinic acid (PA1) (chlorogenic acid) | $C_{16}H_{18}O_{9}$ | *SM* |
| 4-O-caffeoylquinic acid (PA3) | $C_{16}H_{18}O_{9}$ | *SM* |
| 5-O-feruloylquinic acid (PA4) | $C_{17}H_{20}O_{9}$ | *SM* |

| | | |
|---|---|---|
| 1,5-O- dicaffeoylquinic acid (PA6) | $C_{25}H_{24}O_{12}$ | *SM* |
| 3,5-O- dicaffeoylquinic acid (PA5) | $C_{25}H_{24}O_{12}$ | *SM* |
| 4,5-O-dicaffeoylquinic acid (PA7) | $C_{25}H_{24}O_{12}$ | *SM* |
| cynarin | $C_{25}H_{24}O_{12}$ | *SM* |
| mariamide A | $C_{42}H_{46}N_4O_{10}$ | *SM* |
| mariamide B | $C_{21}H_{24}N_2O_5$ | *SM* |
| 3- methylcarboxymethyl-indole-1-N-beta-D-glucopyranoside | $C_{16}H_{19}NO_7$ | *SM* |
| angeloylgomisin H | $C_{28}H_{36}O_8$ | *SCH* |
| angeloylgomisin P | $C_{28}H_{34}O_9$ | *SCH* |
| angeloylgomisin Q | $C_{29}H_{38}O_9$ | *SCH* |
| benzoylgomisin H | $C_{30}H_{34}O_8$ | *SCH* |
| benzoylgomisin O | $C_{30}H_{32}O_8$ | *SCH* |
| gomisin A | $C_{23}H_{28}O_7$ | *SCH* |
| gomisin B | $C_{28}H_{34}O_9$ | *SCH* |
| gomisin D | $C_{28}H_{34}O_{10}$ | *SCH* |
| gomisin F | $C_{28}H_{34}O_9$ | *SCH* |
| gomisin G | $C_{30}H_{32}O_9$ | *SCH* |
| gomisin J | $C_{22}H_{28}O_6$ | *SCH* |
| gomisin K1, K2, K3 | $C_{23}H_{30}O_6$ | *SCH* |
| gomisin M1, M2, L1, L2 | $C_{22}H_{26}O_6$ | *SCH* |
| gomisin N | $C_{23}H_{28}O_6$ | *SCH* |
| isoschisandrin | $C_{24}H_{32}O_7$ | *SCH* |
| propinquanin F | $C_{28}H_{36}O_8$ | *SCH* |
| schisandrin | $C_{24}H_{32}O_7$ | *SCH* |
| schisandrin A | $C_{24}H_{32}O_6$ | *SCH* |
| schisandrin B | $C_{23}H_{28}O_6$ | *SCH* |
| schisandrin C | $C_{22}H_{24}O_6$ | *SCH* |
| schisantherin A | $C_{30}H_{32}O_9$ | *SCH* |
| schisantherin C | $C_{28}H_{34}O_9$ | *SCH* |
| tigloylgomisin P | $C_{28}H_{34}O_9$ | *SCH* |

| | | |
|---|---|---|
| adenosine | $C_{10}H_{13}N_5O_4$ | *CS* |
| cordycedipeptide A | $C_9H_{14}N_3O_3$ | *CS* |
| cordycepic acid | $C_6H_{14}O_6$ | *CS* |
| cordycepin | $C_{10}H_{13}N_5O_3$ | *CS* |
| cordypyridone A | $C_{16}H_{23}NO_3$ | *CS* |
| cordypyridone B | $C_{16}H_{23}NO_3$ | *CS* |
| dipicolinic acid | $C_7H_5NO_4$ | *CS* |
| farinosone A | $C_{25}H_{27}NO_4$ | *CS* |
| farinosone B | $C_{25}H_{26}NO_5$ | *CS* |
| farinosone C | $C_{19}H_{25}NO_5$ | *CS* |
| hypoxanthine | $C_5H_4N_4O$ | *CS* |
| macrolides | $C_{10}H_{14}O_4$ | *CS* |
| militarinone A | $C_{26}H_{37}NO_6$ | *CS* |
| militarinone B | $C_{26}H_{33}NO_5$ | *CS* |
| militarinone C | $C_{26}H_{33}NO_4$ | *CS* |
| militarinone D | $C_{26}H_{31}NO_4$ | *CS* |
| myriocin | $C_{21}H_{39}NO_6$ | *CS* |
| N-acetylgalactosamine | $C_8H_{15}NO_6$ | *CS* |
| naphthaquinone | $C_{10}H_6O_2$ | *CS* |
| paecilomycine A | $C_{15}H_{22}O_4$ | *CS* |
| paecilomycine B | $C_{15}H_{22}O_5$ | *CS* |
| paecilomycine C | $C_{15}H_{20}O_4$ | *CS* |
| paecilosetin | $C_{22}H_{31}NO_4$ | *CS* |
| spirotenuipesine A | $C_{15}H_{22}O_4$ | *CS* |
| spirotenuipesine B | $C_{15}H_{22}O_5$ | *CS* |
| 2-(4-hydroxy phenyl) ethyl-O-beta-D- glucopyranoside | $C_{14}H_{20}O_7$ | *SB* |
| apigenin 7-O-glucoside | $C_{21}H_{20}O_{10}$ | *SB* |
| baicalein | $C_{15}H_{10}O_5$ | *SB* |
| baicalin | $C_{21}H_{18}O_{11}$ | *SB* |
| caffeic acid | $C_9H_8O_4$ | *SB* |

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|---|---|---|
| isomartynoside | $C_{31}H_{40}O_{15}$ | *SB* |
| martynoside | $C_{31}H_{40}O_{15}$ | *SB* |
| neobaicalein (skullcapflavone II) | $C_{19}H_{18}O_8$ | *SB* |
| oroxylin A | $C_{16}H_{12}O_5$ | *SB* |
| oroxylin A glucoronide | $C_{22}H_{20}O_{11}$ | *SB* |
| skullcapflavone I | $C_{17}H_{14}O_6$ | *SB* |
| skullcapflavone I 2'-O-glucoside | $C_{23}H_{24}O_{11}$ | *SB* |
| ursolic acid | $C_{30}H_{48}O_3$ | *SB* |
| verbascoside | $C_{29}H_{36}O_{15}$ | *SB* |
| wogonin | $C_{16}H_{12}O_5$ | *SB* |
| wogonoside | $C_{22}H_{20}O_{11}$ | *SB* |
| cinnamaldehyde | $C_9H_8O$ | *CB* |
| fenchone | $C_{10}H_{16}O$ | *CB* |
| citral | $C_{10}H_{16}O$ | *CB* |
| salonitenolide | $C_{15}H_{20}O_4$ | *CB* |
| cnicin | $C_{20}H_{26}O_7$ | *CB* |
| arctigenin | $C_{21}H_{24}O_6$ | *CB* |
| trachelogenin | $C_{21}H_{24}O_7$ | *CB* |
| nortracheloside | $C_{26}H_{32}O_{12}$ | *CB* |
| absinthin | $C_{30}H_{40}O_6$ | *CB* |
| alpha-amyrenone | $C_{30}H_{48}O$ | *CB* |
| alpha-amyrine | $C_{30}H_{50}O$ | *CB* |
| alpha-amyrin acetate | $C_{32}H_{52}O_2$ | *CB* |
| multiflorenol acetate | $C_{32}H_{52}O_2$ | *CB* |
| p-anisaldehyde | $C_8H_8O_2$ | *FV* |
| trans-anethole | $C_{10}H_{12}O$ | *FV* |
| estragole | $C_{10}H_{12}O$ | *FV* |
| fenchone | $C_{10}H_{16}O$ | *FV* |
| kaempferol | $C_{15}H_{10}O_6$ | *FV* |
| naringenin | $C_{15}H_{12}O_5$ | *FV* |

| | | |
|---|---|---|
| acacetin | $C_{16}H_{12}O_5$ | *FV* |
| isorhamnetin | $C_{16}H_{12}O_7$ | *FV* |
| photoanethole | $C_{16}H_{16}O_2$ | *FV* |
| 3-O-caffeoylquinic acid | $C_{16}H_{18}O_9$ | *FV* |
| 4-O-caffeoylquinic acid | $C_{16}H_{18}O_9$ | *FV* |
| 5-O-caffeoylquinic acid | $C_{16}H_{18}O_9$ | *FV* |
| sinapyl glucoside | $C_{17}H_{22}O_9$ | *FV* |
| rosmarinic acid | $C_{18}H_{16}O_8$ | *FV* |
| dianethole | $C_{19}H_{22}O_2$ | *FV* |
| trans-resveratrol-3-O-beta-d-glucopyranoside | $C_{20}H_{22}O_8$ | *FV* |
| kampferol-3-O-glucuronide | $C_{21}H_{18}O_{12}$ | *FV* |
| quercetin-3-O-glucuronide | $C_{21}H_{18}O_{13}$ | *FV* |
| kaempferol-3-O-glucoside | $C_{21}H_{20}O_{11}$ | *FV* |
| quercetin-3-O-galactoside (hyperoside) | $C_{21}H_{20}O_{12}$ | *FV* |
| isoquercetin | $C_{21}H_{20}O_{12}$ | *FV* |
| isorhamnetin-3-O-glucoside | $C_{22}H_{22}O_{12}$ | *FV* |
| syringin-4-O-beta-glucoside | $C_{23}H_{34}O_{14}$ | *FV* |
| 1,3-O-di-caffeoylquinic acid | $C_{25}H_{24}O_{12}$ | *FV* |
| 1,4-O-di-caffeoylquinic acid | $C_{25}H_{24}O_{12}$ | *FV* |
| 1,5-O-di-caffeoylquinic acid | $C_{25}H_{24}O_{12}$ | *FV* |
| kaempferol-3-O-rutinoside | $C_{27}H_{30}O_{15}$ | *FV* |
| eriodictyol-7-rutinoside | $C_{27}H_{32}O_{15}$ | *FV* |
| cis a trans-miyabenol C | $C_{42}H_{32}O_9$ | *FV* |
| gallic acid | $C_7H_6O_5$ | *TO* |
| esculetin | $C_9H_6O_4$ | *TO* |
| caffeic acid | $C_9H_8O_4$ | *TO* |
| apigenin | $C_{15}H_{10}O_5$ | *TO* |
| luteolin | $C_{15}H_{10}O_6$ | *TO* |
| quercetin | $C_{15}H_{10}O_7$ | *TO* |
| taraxinic acid | $C_{15}H_{18}O_4$ | *TO* |

| | | |
|---|---|---|
| coumestrol | $C_{15}H_8O_5$ | *TO* |
| chlorogenic acid | $C_{16}H_{18}O_9$ | *TO* |
| artemetin | $C_{20}H_{20}O_8$ | *TO* |
| luteolin-7-O-beta-D-glucopyranoside (cyranoside) | $C_{21}H_{20}O_{11}$ | *TO* |
| isoquercetin | $C_{21}H_{20}O_{12}$ | *TO* |
| beta-amyrin | $C_{30}H_{50}O$ | *TO* |
| taraxerol | $C_{30}H_{50}O$ | *TO* |
| taraxasterol | $C_{30}H_{50}O$ | *TO* |
| taraxasteryl acetate | $C_{32}H_{52}O_2$ | *TO* |
| lutein epoxide | $C_{40}H_{56}O_3$ | *TO* |
| lutein | $C_{40}H_{56}O_2$ | *TO* |
| 4-methyl coumarin | $C_{10}H_8O_2$ | *GG* |
| liqcoumarin | $C_{12}H_{10}O_4$ | *GG* |
| quercetin | $C_{15}H_{10}O_7$ | *GG* |
| liquiritigenin | $C_{15}H_{12}O_4$ | *GG* |
| isoliquiritigenin | $C_{15}H_{12}O_4$ | *GG* |
| glyzaglabrin | $C_{16}H_{10}O_6$ | *GG* |
| formononetin | $C_{16}H_{12}O_4$ | *GG* |
| 7-methoxy-2-methylisoflavone | $C_{17}H_{14}O_3$ | *GG* |
| 7-acetoxy-2-methyl-isoflavone | $C_{18}H_{14}O_4$ | *GG* |
| glyzarin | $C_{18}H_{14}O_4$ | *GG* |
| licoisoflavone B | $C_{20}H_{16}O_6$ | *GG* |
| glabrene | $C_{20}H_{18}O_4$ | *GG* |
| licoflavonol | $C_{20}H_{18}O_6$ | *GG* |
| licoisoflavone A | $C_{20}H_{18}O_6$ | *GG* |
| glabridin | $C_{20}H_{20}O_4$ | *GG* |
| quercetin-3-glucoside | $C_{21}H_{20}O_{12}$ | *GG* |
| isoliquiritin | $C_{21}H_{22}O_9$ | *GG* |
| liquiritoside (liquiritin) | $C_{21}H_{22}O_9$ | *GG* |
| glabrol | $C_{25}H_{28}O_4$ | *GG* |

| | | |
|---|---|---|
| licuraside | $C_{26}H_{30}O_{13}$ | *GG* |
| isoglabrolide | $C_{30}H_{44}O_4$ | *GG* |
| glabrolide | $C_{30}H_{44}O_4$ | *GG* |
| liquoric acid | $C_{30}H_{44}O_5$ | *GG* |
| liquiritic acid | $C_{30}H_{46}O_4$ | *GG* |
| glycyrrhetinic acid (enoxolone) | $C_{30}H_{46}O_4$ | *GG* |
| glycyrrhizin | $C_{42}H_{62}O_{16}$ | *GG* |
| licoagrone | $C_{45}H_{42}O_{10}$ | *GG* |


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**Supplementary Table 2** Characteristics of the bioactive compounds identified by the U-HPLC-HRMS/MS targeted screening.

| Searched compound[a] | Elemental composition | Neutral exact mass (m/z) | RT (min) | Ionization polarity | Degree of certainty of compound identification [b] | Overview of the samples in which the compounds were detected[c] | | | | | | | | | | | | | | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | | Silymarin SA | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | 11 | 12 | 13 | 14 | 15 | 16 | 17 | 18 | 19 | 20 | 21 | 22 | 23 | 24 | 25 | 26 |
| isosilandrin A,B; neosilyhermin A,B; silandrin A,B; silyhermin, silymonin | C25H22O9 | 466.1264 | 3.42 | POS | 2 | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| | | | 3.72 | POS | 2 | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| | | | 3.82 | POS | 2 | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| | | | 4.45 | POS | 2 | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| | | | 5.13 | NEG | 2 | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| | | | 5.85 | NEG | 2 | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| | | | 6.47 | NEG | 2 | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| | | | 6.57 | NEG | 2 | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| | | | 6.69 | NEG | 2 | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| | | | 6.94 | NEG | 2 | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| silyamandin | C25H22O11 | 498.1162 | 3.80 | NEG | 2 | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| | | | 4.80 | POS | 2 | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| | | | 5.16 | NEG | 2 | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| catechin, epicatechin | C15H14O6 | 290.0790 | 3.28 | NEG | 1 | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| | | | 3.77 | NEG | 2 | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| | | | 4.79 | NEG | 2 | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| | | | 5.60 | NEG | 2 | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| naringenin | C15H12O5 | 272.0685 | 3.77 | NEG | 2 | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| | | | 4.59 | NEG | 2 | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| | | | 5.14 | POS | 2 | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| | | | 5.88 | NEG | 1 | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| | | | 6.09 | NEG | 2 | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| | | | 6.58 | NEG | 2 | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| | | | 7.98 | NEG | 2 | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| aromadendrin, eriodictyol | C15H12O6 | 288.0634 | 4.55 | NEG | 2 | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| | | | 5.28 | NEG | 2 | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| | | | 5.65 | POS | 2 | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| eupatilin | C18H16O7 | 344.0896 | 4.18 | NEG | 2 | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| | | | 4.92 | NEG | 2 | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| | | | 6.46 | NEG | 2 | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| | | | 6.55 | POS | 2 | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| | | | 6.71 | POS | 2 | | | | | | | | | | | | | | | | | | | | | | | | | | | |

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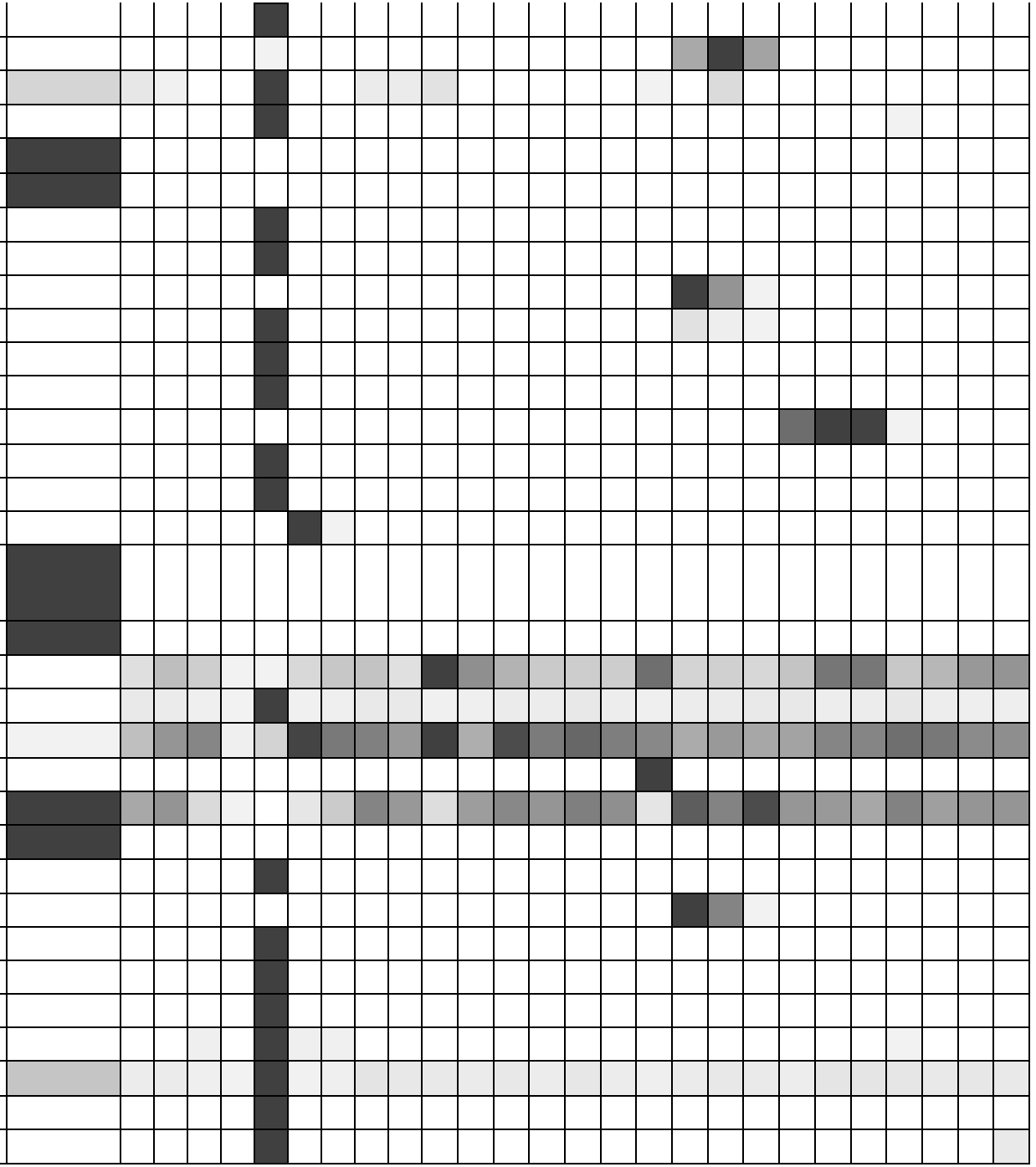
|---|---|---|---|---|---|---|
| | | | 7.75 | POS | 2 | |
| | | | 8.03 | POS | 2 | |
| **hymenoxin** | C19H18O8 | 374.1002 | 6.74 | POS | 2 | |
| | | | 6.96 | POS | 2 | |
| **jaceosidin** | C17H14O7 | 330.0740 | 4.26 | NEG | 2 | |
| | | | 5.32 | POS | 2 | |
| | | | 5.45 | NEG | 2 | |
| | | | 6.07 | POS | 2 | |
| | | | 6.19 | NEG | 2 | |
| | | | 6.42 | POS | 2 | |
| | | | 6.67 | POS | 2 | |
| | | | 6.88 | NEG | 2 | |
| **sudachitin** | C18H16O8 | 360.0845 | 4.18 | NEG | 1 | |
| | | | 5.66 | POS | 2 | |
| | | | 5.75 | NEG | 2 | |
| **vitexin, isovitexin, apigenin-7-O-glucoside** | C21H20O10 | 432.1056 | 4.13 | POS | 2 | |
| | | | 6.41 | NEG | 2 | |
| **luteolin** | C15H10O6 | 286.0477 | 4.01 | NEG | 1 | |
| | | | 5.78 | NEG | 1 | |
| **kaempferol** | C15H10O6 | 286.0477 | 5.26 | POS | 2 | |
| | | | 6.34 | NEG | 2 | |
| | | | 6.88 | NEG | 2 | |
| **pectolinarigenin, kumatakenin** | C17H14O6 | 314.0790 | 3.69 | NEG | 2 | |
| | | | 5.27 | NEG | 2 | |
| | | | 5.75 | NEG | 2 | |
| | | | 6.71 | POS | 2 | |
| | | | 7.10 | NEG | 2 | |
| | | | 7.23 | POS | 2 | |
| | | | 7.55 | NEG | 2 | |
| | | | 5.17 | POS | 2 | |
| **apigenin** | C15H10O5 | 270.0528 | 6.35 | POS | 1 | |
| **genistein** | C15H10O5 | 270.0528 | 5.63 | NEG | 2 | |
| | | | 8.14 | NEG | 2 | |



| | | | | | | |
|---|---|---|---|---|---|---|
| | | | 3.78 | NEG | 2 | |
| **nepetin, rhamentin** | C16H12O7 | 316.0583 | 4.00 | NEG | 2 | |
| | | | 4.27 | NEG | 2 | |
| | | | 4.80 | POS | 2 | |
| | | | 5.63 | NEG | 2 | |
| | | | 6.34 | NEG | 2 | |
| | | | 6.63 | NEG | 2 | |
| | | | 6.74 | POS | 2 | |
| | | | 2.98 | POS | 2 | |
| | | | 3.88 | NEG | 2 | |
| | | | 4.40 | NEG | 2 | |
| **orientin, isoorientin, astragalin, cynaroside** | C21H20O11 | 448.1006 | 3.93 | NEG | 2 | |
| | | | 4.02 | POS | 2 | |
| | | | 4.92 | NEG | 2 | |
| **apigenin-5,7-dimethyl ether** | C17H14O5 | 298.0841 | 5.41 | NEG | 2 | |
| | | | 5.73 | POS | 2 | |
| | | | 6.09 | POS | 2 | |
| | | | 6.50 | POS | 2 | |
| | | | 6.70 | NEG | 2 | |
| | | | 7.76 | NEG | 2 | |
| | | | 5.18 | POS | 2 | |
| | | | 5.59 | POS | 2 | |
| | | | 6.00 | POS | 2 | |
| **apigenin-7-O-glucuronide** | C21H18O11 | 446.0849 | 5.78 | POS | 2 | |
| | | | 4.26 | NEG | 1 | |
| | | | 4.67 | NEG | 2 | |
| **isokaempferide-7-rhamnoside** | C22H22O10 | 446.1213 | 8.79 | POS | 2 | |
| **rutin** | C27H30O16 | 610.1534 | 4.21 | NEG | 2 | |
| | C27H30O15 | 594.1585 | 4.69 | NEG | 2 | |

| | | | | | | |
|---|---|---|---|---|---|---|
| **apigenin-4,7-diglucoside, kaempferol-3-rutinoside** | | | 5.96 | NEG | 2 | |
| **miquelianin** | C21H18O13 | 478.0747 | 6.79 | POS | 2 | |
| **patuletin** | C16H12O8 | 332.0532 | 3.14 | POS | 2 | |
| | | | 3.69 | NEG | 1 | |
| | | | 3.75 | NEG | 2 | |
| **quercetin** | C15H10O7 | 302.0427 | 3.99 | POS | 1 | |
| | | | 4.30 | POS | 2 | |
| | | | 5.61 | NEG | 2 | |
| | | | 5.93 | NEG | 1 | |
| | | | 6.81 | NEG | 2 | |
| | | | 1.80 | POS | 2 | |
| | | | 2.88 | POS | 2 | |
| | | | 2.96 | POS | 2 | |
| **coniferylaldehyd** | C10H10O3 | 178.0630 | 3.56 | NEG | 2 | |
| | | | 4.30 | POS | 2 | |
| | | | 4.87 | POS | 2 | |
| | | | 3.21 | NEG | 2 | |
| | | | 3.56 | NEG | 2 | |
| | | | 4.52 | POS | 2 | |
| **dihydroconiferyl alcohol** | C10H14O3 | 182.0943 | 1.67 | NEG | 2 | |
| | | | 3.03 | NEG | 2 | |
| | | | 3.20 | NEG | 2 | |
| **syringaldehyde** | C9H10O4 | 182.0579 | 3.79 | POS | 2 | |
| | | | 5.01 | NEG | 2 | |
| | | | 5.95 | POS | 2 | |
| | | | 10.20 | POS | 2 | |
| | | | 1.65 | POS | 2 | |
| | | | 3.25 | NEG | 2 | |
| | | | 3.46 | NEG | 2 | |
| **ethyl caffeate, methyl ferulate** | C11H12O4 | 208.0736 | 3.97 | NEG | 2 | |
| | | | 4.22 | POS | 2 | |
| | | | 4.87 | NEG | 2 | |

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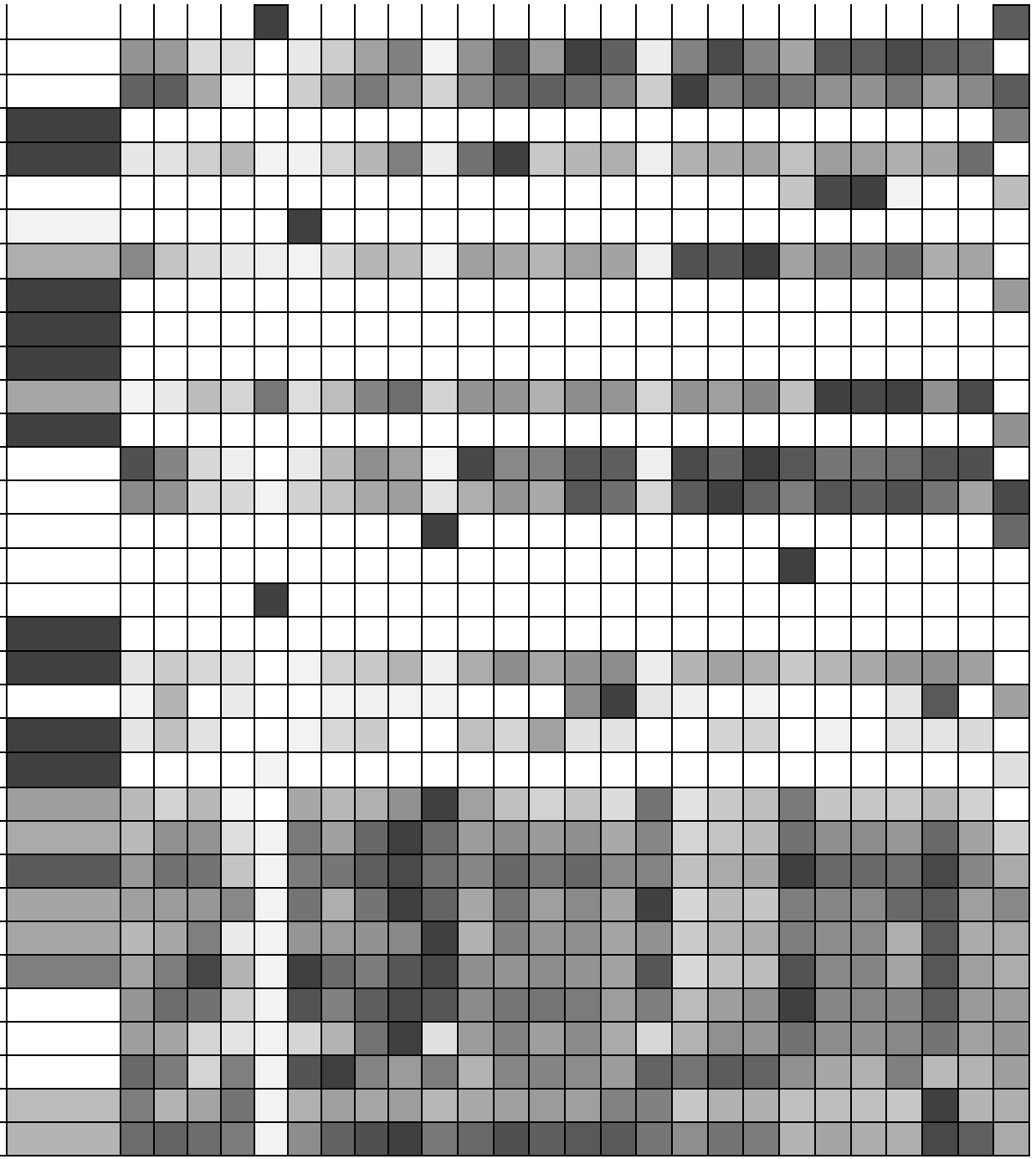
|---|---|---|---|---|---|---|
| | | | 5.30 | NEG | 2 | |
| | | | 5.71 | NEG | 2 | |
| | | | 5.89 | POS | 2 | |
| | | | 5.97 | NEG | 2 | |
| | | | 7.09 | POS | 2 | |
| | | | 4.27 | NEG | 2 | |
| | | | 4.59 | NEG | 2 | |
| | | | 1.65 | NEG | 2 | |
| **1,5-O-dicaffeoylquinic acid, 3,5-O-dicaffeoylquinic acid, 4,5-O-dicaffeoylquinic acid, cynarin** | C25H24O12 | 516.1268 | 3.19 | NEG | 2 | |
| | | | 3.61 | NEG | 2 | |
| **5-O-feruloylquinic acid** | C17H20O9 | 368.1107 | 3.29 | NEG | 1 | |
| | | | 3.36 | POS | 2 | |
| | | | 4.95 | POS | 2 | |
| **caffeic acid** | C9H8O4 | 180.0423 | 8.69 | POS | 2 | |
| | | | 1.73 | POS | 2 | |
| | | | 3.64 | NEG | 1 | |
| | | | 6.94 | NEG | 2 | |
| **coumaric acid** | C9H8O3 | 164.0473 | 5.37 | NEG | 1 | |
| | | | 3.57 | NEG | 1 | |
| | | | 3.20 | NEG | 1 | |
| | | | 3.11 | POS | 2 | |
| **dihydroxybenzoic acid** | C7H6O4 | 154.0266 | 3.24 | NEG | 2 | |
| | | | 4.10 | NEG | 2 | |
| **ferulic acid** | C10H10O4 | 194.0579 | 4.94 | NEG | 2 | |
| | | | 5.51 | POS | 2 | |
| | | | 1.33 | NEG | 1 | |
| | | | 2.37 | POS | 2 | |
| | | | 2.98 | POS | 2 | |
| **gallic acid** | C7H6O5 | 170.0215 | 4.05 | NEG | 2 | |
| | | | 4.74 | POS | 2 | |

| | | | | | | |
|---|---|---|---|---|---|---|
| | | | 2.99 | NEG | 2 | |
| | | | 4.13 | POS | 2 | |
| | | | 5.92 | POS | 2 | |
| **guaiacol** | C7H8O2 | 124.0524 | 1.88 | NEG | 2 | |
| | | | 3.08 | NEG | 1 | |
| | | | 3.88 | NEG | 2 | |
| **chlorogenic acid** | C16H18O9 | 354.0951 | 1.65 | POS | 2 | |
| | | | 2.75 | NEG | 1 | |
| | | | 3.00 | NEG | 2 | |
| **salicylic acid** | C7H6O3 | 138.0317 | 3.19 | NEG | 2 | |
| | | | 3.90 | NEG | 2 | |
| | | | 4.55 | NEG | 2 | |
| | | | 3.56 | NEG | 2 | |
| | | | 4.12 | POS | 2 | |
| | | | 4.50 | NEG | 2 | |
| **sinapinic acid** | C11H12O5 | 224.0685 | 1.64 | NEG | 2 | |
| | | | 2.86 | POS | 2 | |
| | | | 4.03 | NEG | 2 | |
| **syringic acid** | C9H10O5 | 198.0528 | 1.48 | POS | 2 | |
| | | | 1.65 | NEG | 1 | |
| | | | 3.02 | POS | 2 | |
| **vanillic acid** | C8H8O4 | 168.0423 | 3.16 | POS | 2 | |
| | | | 3.34 | POS | 2 | |
| | | | 4.69 | POS | 2 | |
| | | | 4.89 | POS | 2 | |
| | | | 5.05 | POS | 2 | |
| **mariamide A** | C42H46N4O10 | 766.3214 | 5.24 | POS | 2 | |
| | | | 5.36 | POS | 2 | |
| | | | 5.45 | POS | 2 | |
| | | | 5.69 | POS | 2 | |
| | | | 6.04 | POS | 2 | |
| | | | 14.82 | POS | 2 | |
| | | | 4.32 | POS | 2 | |
| | | | 4.65 | POS | 2 | |

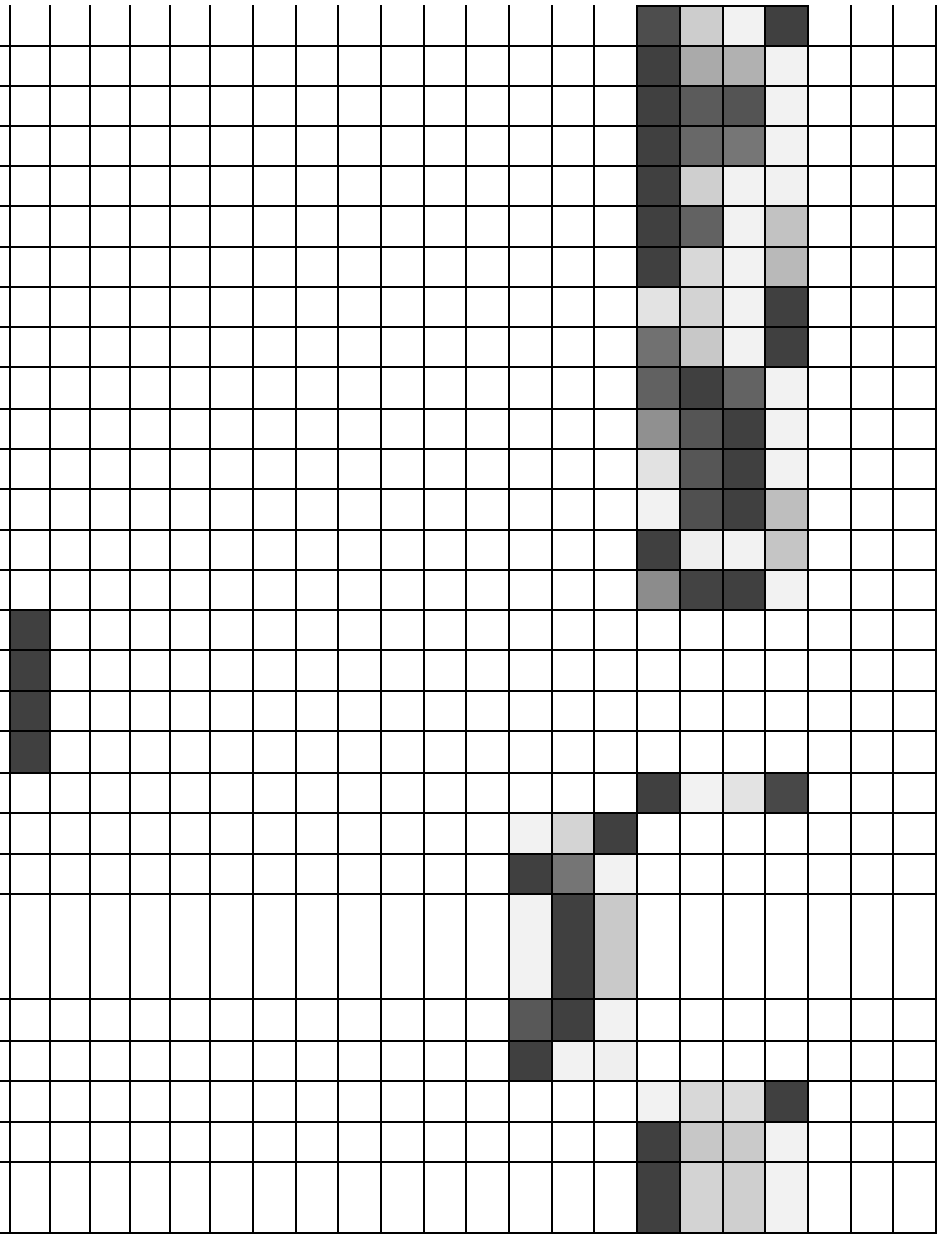


| | | | | | | |
|---|---|---|---|---|---|---|
| | | | 5.00 | POS | 2 | |
| **mariamide B** | C21H24N2O5 | 384.1685 | 3.53 | POS | 2 | |
| | | | 3.34 | POS | 2 | |
| | | | 7.71 | POS | 2 | |
| **3-methylcarboxymethyl-indole-1-N-beta-D-glucopyranoside** | C16H19NO7 | 337.1162 | 8.00 | POS | 2 | |
| **naphthaquinone** | C10 H6 O2 | 158.0368 | 9.09 | NEG | 2 | |
| **angeloylgomisin H, propinquanin F** | C28 H36 O8 | 500.2410 | 7.97 | POS | 2 | |
| | | | 8.15 | POS | 2 | |
| | | | 8.36 | POS | 2 | |
| **angeloylgomisin P, gomisin B, gomisin F, schisantherin C, tigloylgomisin P** | C28 H34 O9 | 514.2203 | 8.46 | POS | 2 | |
| | | | 8.59 | POS | 2 | |
| | | | 8.79 | POS | 2 | |
| | | | 9.11 | POS | 2 | |
| | | | 7.86 | POS | 2 | |
| | | | 8.06 | POS | 2 | |
| | | | 7.71 | POS | 2 | |
| **angeloylgomisin Q** | C29 H38 O9 | 530.2516 | 8.00 | POS | 2 | |
| | | | 7.76 | POS | 2 | |
| **benzoylgomisin H** | C30 H34 O8 | 522.2254 | 8.44 | POS | 2 | |
| | | | 9.09 | NEG | 2 | |
| **gomisin A** | C23 H28 O7 | 416.1835 | 6.69 | POS | 2 | |
| | | | 7.34 | POS | 2 | |
| | | | 8.07 | POS | 2 | |
| **gomisin D** | C28 H34 O10 | 530.2152 | 8.64 | POS | 2 | |
| | | | 7.90 | POS | 2 | |
| **gomisin G, schisantherin A** | C30 H32 O9 | 536.2046 | 8.27 | POS | 2 | |
| | | | 8.37 | NEG | 2 | |
| **gomisin J** | C22 H28 O6 | 388.1886 | 8.53 | POS | 2 | |

| | | | | | | |
|---|---|---|---|---|---|---|
| | | | 8.81 | POS | 2 | |
| | | | 8.98 | POS | 2 | |
| | | | 9.19 | POS | 2 | |
| **gomisin K1, K2, K3** | C23 H30 O6 | 402.2042 | 9.26 | POS | 2 | |
| | | | 9.46 | POS | 2 | |
| **gomisin M1, M2, L1, L2** | C22 H26 O6 | 386.1729 | 9.57 | POS | 2 | |
| | | | 8.01 | POS | 2 | |
| | | | 8.20 | POS | 2 | |
| | | | 10.17 | POS | 2 | |
| **gomisin N, schisandrin B** | C23 H28 O6 | 400.1886 | 10.27 | POS | 2 | |
| | | | 9.52 | POS | 2 | |
| | | | 9.11 | NEG | 2 | |
| | | | 10.85 | POS | 2 | |
| **schisandrin A** | C24 H32 O6 | 416.2199 | 6.67 | POS | 2 | |
| **schisandrin C** | C22 H24 O6 | 384.1573 | 7.06 | POS | 2 | |
| | | | 7.76 | POS | 2 | |
| **schisandrin, isoschisandrin** | C24 H32 O7 | 432.2148 | 5.62 | POS | 2 | |
| | | | 5.95 | POS | 2 | |
| | | | 6.31 | POS | 2 | |
| **trachelogenin** | C21 H24 O7 | 388.1522 | 5.84 | POS | 2 | |
| | | | 4.10 | POS | 2 | |
| | | | 3.96 | POS | 2 | |
| **arctigenin** | C21 H24 O6 | 372.1573 | 4.18 | NEG | 2 | |
| **nortracheloside** | C26 H32 O12 | 536.1894 | 5.74 | POS | 2 | |
| **rosmarinic acid** | C18 H16 O8 | 360.0845 | 5.98 | POS | 2 | |
| | | | 7.10 | NEG | 2 | |
| | | | 0.73 | NEG | 2 | |
| | | | 5.19 | POS | 1 | |
| | | | 5.40 | POS | 2 | |
| **cordycepic acid** | C6 H14 O6 | 182.0790 | 5.63 | NEG | 2 | |
| **baicalein** | C15 H10 O5 | 270.0528 | 6.39 | NEG | 2 | |
| | | | 6.73 | POS | 2 | |

| | | | | | | |
|---|---|---|---|---|---|---|
| | | | 6.96 | POS | 2 | |
| | | | 5.37 | NEG | 2 | |
| **neobaicalein** | C19 H18 O8 | 374.1002 | 5.75 | NEG | 2 | |
| | | | 5.97 | NEG | 2 | |
| **skullcapflavone I** | C17 H14 O6 | 314.0790 | 7.10 | NEG | 2 | |
| | | | 7.23 | POS | 2 | |
| | | | 7.55 | NEG | 2 | |
| | | | 5.41 | POS | 2 | |
| | | | 7.38 | POS | 2 | |
| | | | 7.57 | POS | 2 | |
| **oroxylin A, wogonin** | C16 H12 O5 | 284.0685 | 5.22 | NEG | 1 | |
| | | | 5.58 | NEG | 1 | |
| | | | 5.86 | POS | 2 | |
| **baicalin** | C21 H18 O11 | 446.0849 | 5.93 | NEG | 2 | |
| | | | 5.68 | POS | 2 | |
| | | | 5.86 | POS | 2 | |
| | | | 6.13 | POS | 2 | |
| **oroxylin A glucoronide, wogonoside** | C22 H20 O11 | 460.1006 | 6.70 | POS | 1 | |
| | | | 9.12 | NEG | 2 | |
| **skullcapflavone I 2-O-glucoside** | C23 H24 O11 | 476.1319 | 9.69 | NEG | 2 | |
| **isorhamnetin** | C16 H12 O7 | 316.0583 | 5.19 | POS | 1 | |
| **7-acetoxy-2-methyl-isoflavone, glyzarin** | C18 H14 O4 | 294.0892 | 6.86 | POS | 1 | |
| | | | 8.60 | POS | 2 | |
| **formononetin** | C16 H12 O4 | 268.0736 | 8.72 | NEG | 2 | |
| | | | 8.97 | NEG | 2 | |
| **licoisoflavone B** | C20 H16 O6 | 352.0947 | 9.10 | NEG | 2 | |
| | | | 4.85 | POS | 2 | |
| | | | 7.98 | NEG | 2 | |
| | | | 8.17 | NEG | 2 | |
| **glabrene** | C20 H18 O4 | 322.1205 | 8.61 | NEG | 2 | |
| | | | 9.13 | NEG | 2 | |

| | | | | | | |
|---|---|---|---|---|---|---|
| | | | 9.30 | NEG | 2 | |
| | | | 9.72 | NEG | 2 | |
| | | | 7.65 | NEG | 2 | |
| | | | 8.15 | NEG | 2 | |
| | | | 9.20 | NEG | 2 | |
| **glabridin** | C20 H20 O4 | 324.1362 | 9.38 | NEG | 2 | |
| | | | 9.71 | NEG | 2 | |
| | | | 10.68 | POS | 2 | |
| | | | 11.15 | NEG | 2 | |
| **glabrol** | C25 H28 O4 | 392.1988 | 8.75 | NEG | 2 | |
| | | | 9.19 | NEG | 2 | |
| | | | 4.96 | NEG | 2 | |
| **licoflavonol, licoisoflavone A** | C20 H18 O6 | 354.1103 | 5.13 | NEG | 2 | |
| | | | 3.96 | POS | 2 | |
| **licuraside** | C26 H30 O13 | 550.1686 | 4.12 | POS | 1 | |
| | | | 4.96 | POS | 2 | |
| **isoliquiritigenin** | C15 H12 O4 | 256.0736 | 5.30 | POS | 2 | |
| | | | 4.12 | NEG | 2 | |
| **martynoside, isomartynoside** | C31 H40 O15 | 652.2367 | 4.42 | NEG | 2 | |
| | | | 3.04 | POS | 2 | |
| **verbascoside** | C29 H36 O15 | 624.2054 | 4.55 | POS | 2 | |
| | | | 5.20 | NEG | 2 | |
| **syringin-4-O-beta-glucoside** | C23 H34 O14 | 534.1949 | 5.04 | POS | 2 | |
| **salonitenolide** | C15 H20 O4 | 264.1362 | 5.20 | POS | 2 | |
| | | | 7.45 | POS | 2 | |
| **cnicin** | C20 H26 O7 | 378.1679 | 15.31 | NEG | 2 | |
| | | | 10.71 | POS | 2 | |
| **fenchone, citral** | C10 H16 O | 152.1201 | 11.63 | NEG | 1 | |



| | | | | | | |
|---|---|---|---|---|---|---|
| **alpha-amyrine, beta-amyrine, taraxerol, taraxasterol** | C30 H50 O | 426.3862 | 11.84 | NEG | 1 | |
| **liquiritic acid, glycyrrhetinic acid** | C30 H46 O4 | 470.3396 | 13.71 | POS | 2 | |
| **ursolic acid** | C30 H48 O3 | 456.3603 | 8.09 | NEG | 2 | |
| | | | 8.40 | NEG | 2 | |
| **glabrolide, isoglabrolide** | C30 H44 O4 | 468.3240 | 3.48 | NEG | 2 | |
| **glycyrrhizin** | C42 H62 O16 | 822.4038 | 4.85 | POS | 2 | |
| | | | | | | |
| **methylcoumarin** | C10 H8 O2 | 160.0524 | | | | |
| | | | | | | |

**Supplementary Table 3** Correlation coefficients ($R^2$)[a] of dependence of antioxidant activity of 26 dietary supplements on U-HPLC-HRMS/MS responses[b] of non-silymarin bioactive compounds present in *Silybum marianum*.

| | | | Potential identity (compound from database) | CAA | ABTS | ORAC | DPPH |
|---|---|---|---|---|---|---|---|
| Phenolics | Simple phenolics | | 1,5-O- dicaffeoylquinic acid; 3,5-O-dicaffeoylquinic acid; 4,5-O-dicaffeoylquinic acid; 5-O-feruloylquinic acid; caffeic acid; coniferylaldehyd; coumaric acid; cynarin; dihydroconiferyl alcohol; dihydroxybenzoic acid; ethyl caffeate; ferulic acid; gallic acid; guaiacol; chlorogenic acid; mariamide A,B; methyl ferulate; salicylic acid; sinapinic acid; syringaldehyde; syringic acid; vanillic acid | 0.543[a] | 0.374 | 0.118 | 0.453 |
| | Flavonoids | flavone/flavonol aglycones | apigenin; apigenin-5,7-dimethyl ether; kaempferol; kumatakenin; luteolin; nepetin; patuletin; pectolinarigenin; quercetin; rhamentin | 0.122 | -0.189 | -0.642 | 0.472 |
| | | flavone/flavonol glycosides | apigenin-4,7-diglucoside; apigenin-7-O-glucoside; apigenin-7-O-glucuronide; astragalin; cynaroside; | 0.221 | -0.051 | -0.052 | 0.339 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| | | | isokaempferide-7-rhamnoside; isoorientin; isovitexin; kaempferol-3-rutinoside; miquelianin; orientin; rutin; vitexin | | | | |
| | | flavonolignans | isosilandrin A,B; neosilyhermin A,B; silandrin A,B; silyamandin; silyhermin; silymonin | 0.277 | 0.420 | -0.246 | 0.446 |
| | | isoflavone | genistein | -0.380 | 0.045 | 0.740 | 0.165 |
| | SUM of flavone/flavonol aglycones and glycosides | | | 0.201 | -0.139 | -0.409 | 0.465 |
| | SUM of flavone/flavonol aglycones and glycosides and isoflavonoids | | | 0.204 | -0.139 | -0.411 | 0.466 |
| | SUM of flavonoids | | | 0.363 | 0.045 | -0.518 | 0.599[a] |
| | SUM of phenolics | | | 0.647[a] | 0.332 | -0.171 | 0.607[a] |
| Alkaloids | | | 3- methylcarboxymethyl-indole-1-N-beta-D-glucopyranoside | 0.520[a] | 0.232 | -0.445 | 0.232 |

[a] Correlation coefficient confirms ($\alpha$=0.05) that the results of antioxidant assay linearly depend on U-HPLC-HRMS/MS responses of non-silymarin antioxidants present in *Silybum marianum* (ABTS df=14, critical value=0.497; ORAC df=19, critical value=0.433; DPPH df=20, critical value=0.423; CAA df=15, critical value=0.482).

[b] For the non-silymarin antioxidants, the analytical standards were not available, so we correlated the sum of areas of the peaks of U-HPLC-HRMS/MS chromatograms.

**Supplementary Table 4** Correlation coefficients ($R^2$) of dependence of antioxidant activity of 26 dietary supplements on U-HPLC-HRMS/MS responses[b] of non-silymarin bioactive compounds present in other plants - *Schisandra chinensis, Cordyceps sinensis, Scutellaria baicalensis, Cnicus benedictus, Foeniculum vulgare, Taraxacum officinale* and *Glycyrrhiza glabra*.

| | | | **Potential identity (compound from database)** | **$R^2$** | | | | **critical value** | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | CAA | ABTS | ORAC | DPPH | CAA | ABTS | ORAC | DPPH |
| Phenolics | Simple phenolics | | cordycepic acid; isomartynoside; martynoside; naphthaquinone; rosmarinic acid; syringin-4-O-beta-glucoside; verbascoside | 0.194 | -0.745 | -0.546 | -0.593 | 0.95 | 0.95 | 0.95 | 0.95 |
| | Coumarins | | methylcoumarin | -0.604 | -0.218 | -0.100 | -0.451 | 0.497 | 0.433 | 0.423 | 0.482 |
| | Lignans | lignans | angeloylgomisin H; angeloylgomisin P; angeloylgomisin Q; arctigenin; benzoylgomisin H; gomisin A,B,DF,G,J,K1,K2,K3,L1,L2,M1,M2,N; isoschisandrin; propinquanin F; schisandrin A,B,C; schisantherin A,C; tigloylgomisin P; trachelogenin | -0.375 | -0.302 | 0.019 | 0.030 | 0.497 | 0.433 | 0.423 | 0.482 |
| | | lignan glycosides | nortracheloside | 0.963 | -0.995 | 0.998[a] | 0.919 | 0.997 | 0.997 | 0.997 | 0.997 |
| | SUM of lignans and lignan glycosides | | | -0.390 | -0.305 | 0.017 | 0.029 | 0.497 | 0.433 | 0.423 | 0.482 |
| | Flavonoids | flavones/flavonols | baicalein; glabrol; isorhamnetin; neobaicalein; oroxylin A; skullcapflavone I; wogonin | 0.048 | -0.029 | -0.351 | 0.240 | 0.497 | 0.433 | 0.433 | 0.497 |
| | | isoflavonoids | 7-acetoxy-2-methyl-isoflavone; formononetin; glabrene; glabridin; glyzarin; licoflavonol; licoisoflavone A, B | 0.000 | -0.569 | -0.773 | -0.318 | 0.95 | 0.95 | 0.95 | 0.95 |
| | | chalcones | isoliquiritigenin; licuraside | 0.707 | -0.697 | 0.409 | -0.997 | 0.95 | 0.95 | 0.95 | 0.95 |
| | SUM of flavonoids | | | 0.117 | -0.056 | -0.341 | 0.199 | 0.497 | 0.433 | 0.433 | 0.497 |
| | SUM of phenolics | | | 0.029 | -0.315 | -0.023 | 0.058 | 0.497 | 0.433 | 0.423 | 0.482 |
| Saponins | triterpenoidal | | glabrolide; glycyrrhizin; isoglabrolide | -0.194 | 0.735 | 0.554 | 0.585 | 0.95 | 0.95 | 0.95 | 0.95 |
| Terpenes | mono | | citral; fenchone | -0.983 | 0.983 | -0.989 | -0.949 | 0.997 | 0.997 | 0.997 | 0.997 |
| | sesqui | | cnicin; salonitenolide | -0.454 | 0.102 | -0.138 | -0.568 | 0.997 | 0.997 | 0.997 | 0.997 |
| | tri | | alpha,beta-amyrine; glycyrrhetinic acid; liquiritic acid; taraxasterol; taraxerol; ursolic acid | -0.572 | 0.822 | -0.097 | 0.964[a] | 0.95 | 0.95 | 0.95 | 0.950 |

| | | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| SUM of terpenes | -0.596 | -0.893 | -0.606 | -0.726 | 0.754 | 0.754 | 0.754 | 0.754 |

[a] Correlation coefficient confirms ($\alpha$=0.05) that the results of antioxidant assay linearly depend on U-HPLC-HRMS/MS responses of non-silymarin antioxidants present in other plants - *Schisandra chinensis*, *Cordyceps sinensis, Scutellaria baicalensis*, *Cnicus benedictus*, *Foeniculum vulgare*, *Taraxacum officinale* and *Glycyrrhiza glabra.*

[b] For the non-silymarin antioxidants, the analytical standards were not available, so we correlated the sum of areas of the peaks of U-HPLC-HRMS/MS chromatograms